# Entanglement between two fermionic atoms inside a cylindrical harmonic trap

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We investigate quantum entanglement between two (spin-1/2) fermions inside a cylindrical harmonic trap, making use of the von Neumann entropy for the reduced single particle density matrix as the pure state entanglement measure. We explore the dependence of pair entanglement on the geometry and strength of the trap and on the strength of the pairing interaction over the complete range of the effective BCS to BEC crossover. Our result elucidates an interesting connection between our model system of two fermions and that of two interacting bosons.

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## I. INTRODUCTION

Recent experiments with lattice fermions across Feshbach resonance have raised significant hope for the application of atomic quantum gases to implementations of quantum information processing [1, 2, 3]. These experiments usually begin with the preparation of two fermions into each optical lattice site. Making use of a Feshbach resonance [4], the two-atom scattering length is tuned from a small positive value to the attractive side by varying an external magnetic field. During this process, the motional states of the fermionic atom pair in each lattice site can occupy different Bloch bands, exhibiting new features that need further theoretical explanation [5].

In quantum information science, quantum entanglement is viewed as the enabling resource for its potential power over classical information processing, as in quantum teleportation [6, 7, 8, 9, 10] and cryptography [11, 12, 13]. In this paper, we present a thorough investigation of the pair entanglement of two fermions in a single optical lattice site, approximated as a cylindrical harmonic trap. Similar studies have been carried out in a one dimensional harmonic trap [14] and in a three dimensional spherical harmonic trap [15]. The present study differs in two significant aspects: first, we extend earlier studies to the case of three dimensional cylindrical harmonic traps; second, we allow for the possibility that the two interacting atoms may form a molecular bound state, albeit in the broad resonance regime. In the model to be presented below we will parameterize the two atom interaction using a general formalism commonly adopted in the many body system of BCS to BEC crossover [16, 17, 18, 19]. For a broad Feshbach resonance, where most of the currently employed resonance theories do fall into, the earlier results based on a single channel model are easily recovered by excluding the molecular component.

This paper is organized as follows. First, we present the model system and our formulation, essentially parallel to the development and notations of Ref. [5]. Next, we focus on the broad resonance regime and briefly discuss the molecular component. This paves the way for the discussion of our central result — a thorough investigation of the pair entanglement and its dependence on trap strength and geometry, and on atom-atom interaction strength. Finally, we conclude with a brief summary.

## II. TWO INTERACTING FERMIONIC ATOMS IN A HARMONIC TRAP

Following the successful model proposed in Ref. [5], two fermions are assumed to be located in the same lattice site, which for this study is approximated as a harmonic trap. Each optical lattice site represents an independent system, since the quantum tunnelling, or hopping between neighboring sites, is negligible for deep optical lattice potential of interest. The Hamiltonian for the system of two spin-1/2 fermionic atoms is given by

$$H = \sum_{\mathbf{m}\sigma} E_{\mathbf{m}} a^\dagger_{\mathbf{m}\sigma} a_{\mathbf{m}\sigma} + \bar{\nu} b^\dagger b + \sum_{\mathbf{m},\mathbf{n}} \alpha_{\mathbf{m},\mathbf{n}} \left( a^\dagger_{\mathbf{m}\uparrow} a^\dagger_{\mathbf{n}\downarrow} b + h.c. \right), \quad (1)$$

where $E_{\mathbf{m}} = \sum_{j=x,y,z} \hbar\omega_j (m_j + 1/2)$ is the harmonic oscillator energy for state labelled by $\mathbf{m} = (m_x, m_y, m_z)$ with angular frequencies $(\omega_x, \omega_y, \omega_z)$. $a^\dagger_{\mathbf{m}\sigma}$ is the creation operator for a fermionic atom in the open channel with energy $E_{\mathbf{m}}$ and spin $\sigma$. $b^\dagger$ is the creation operator for the two-atom bound state, a bosonic molecule in the closed channel with its center of mass wave function fixed exactly at the harmonic ground state, a result of the simple approximation that the optical lattice trap potential for the bound state molecule is simply equal to the sum of the trap potentials of the two atoms. $\bar{\nu}$ is the energy difference between the closed channel bosonic molecule and the two fermions in the open channel. $\alpha_{\mathbf{m},\mathbf{n}}$ is the coherent coupling element converting two open channel fermions into a closed channel bosonic molecule, which is defined to contain a common constant prefactor $\alpha$, i.e., $\alpha_{\mathbf{m},\mathbf{n}} = \alpha \langle \mathbf{0}_{\text{c.m.}}, \psi_{\text{rel}} | \mathbf{m}, \mathbf{n} \rangle$ with $|\mathbf{m}\rangle$ being the harmonic

orbital of a single atom. The relative motional part of the molecular ground state, $|\psi_{\rm rel}\rangle$, will be approximated as a contact $\delta(\vec{r})$ function, since it is typically of atomic size [5, 20], much less than other length scales in this problem. Such a simplification contains an ultra-violet divergence that can be removed by a suitable momentum cutoff with a renormalized detuning [20]. An alternative formulation involves the use of the regularized delta function [21]. The cylindrical harmonic trap is characterized by the trap frequencies $\omega_x = \omega_y = \omega_\perp = \omega_z/\lambda$ with $\lambda$ parameterizing the trap aspect ratio. Within this model, the two fermionic atoms in the open channel (of being atoms) at bands $\mathbf{m}$ and $\mathbf{n}$ can be converted into a closed channel bosonic molecule, or vice versa. The eigenstate of Hamiltonian (1) can be expressed as

$$|\Psi\rangle = \left(\beta b^\dagger + \sum_{\mathbf{m},\mathbf{n}} \eta_{\mathbf{m},\mathbf{n}} a^\dagger_{\mathbf{m}\uparrow} a^\dagger_{\mathbf{n}\downarrow}\right)|\text{vac}\rangle, \tag{2}$$

again following Ref. [5]. The various coefficients are determined from the following coupled equations

$$\eta_{\mathbf{m},\mathbf{n}} = \beta \frac{\alpha_{\mathbf{m},\mathbf{n}}}{E - E_{\mathbf{m},\mathbf{n}}}, \tag{3}$$

$$E - \bar{\nu} = \sum_{\mathbf{m},\mathbf{n}} \frac{\alpha^2_{\mathbf{m},\mathbf{n}}}{E - E_{\mathbf{m},\mathbf{n}}}, \tag{4}$$

$$\frac{1}{\beta^2} = 1 + \sum_{\mathbf{m},\mathbf{n}} \frac{\alpha^2_{\mathbf{m},\mathbf{n}}}{(E - E_{\mathbf{m},\mathbf{n}})^2}. \tag{5}$$

As in Ref. [5], the divergence in Eq. (4) can be removed by introducing a cutoff in the summation. Such a procedure will renormalize $\bar{\nu}$ to $\nu^*$. By comparing the free space expression of the energy $E$ (renormalized) to the results of resonance scattering at low energies, the parameters $\nu^*$ and $\alpha$ are then matched to the experimentally relevant parameters $a_s$ and $r_0$, where $a_s$ is the $s$-wave scattering length between fermionic atoms in different internal states and $r_0$ is the effective range. The result is [5]

$$\frac{1}{a_s} = -\frac{\sqrt{2}\nu^*\hbar^2}{m\alpha^2\pi^{7/2}} = -\frac{\nu^*|r_0|m}{2\hbar^2}, \tag{6}$$

where $m$ is the mass of the atom. A dimensionless parameter $x = E/(2\hbar\omega_\perp) - 1 - \lambda/2$ is then introduced, with which the energy quantization condition becomes

$$\sqrt{2\lambda}\left[\frac{d_\perp}{a_s} + \frac{|r_0|}{d_\perp}\left(x + 1 + \frac{\lambda}{2}\right)\right] = -\frac{\lambda}{\sqrt{\pi}} F\left(-\frac{x}{\lambda}, \frac{1}{\lambda}\right), \tag{7}$$

where $d_\perp \equiv \sqrt{\hbar/(m\omega_\perp)}$, and the function on the right hand side of Eq. (7) is defined in Ref. [22]

$$F(u,\eta) = \int_0^\infty dt \left(\frac{\eta e^{-ut}}{\sqrt{1-e^{-t}}(1-e^{-\eta t})} - \frac{1}{t^{3/2}}\right). \tag{8}$$

For a spherical trap this reduces to the well-known result of $F(-x,1) = -2\sqrt{\pi}\,\Gamma(-x)/\Gamma(-x-1/2)$ [23]. Furthermore, if $r_0 = 0$, the energy spectrum and eigenfunctions coincide with the results of two atoms in a harmonic trap as studied previously in Refs. [22, 23]. This is a straightforward conclusion, since for $r_0 = 0$, the current model describes the same physical process quantified by a single $s$-wave parameter $a_s$ [22, 23]. A non-zero $r_0$ as incorporated in Ref. [5] allows for a more general model including both open channel fermions and a closed channel bosonic molecule.

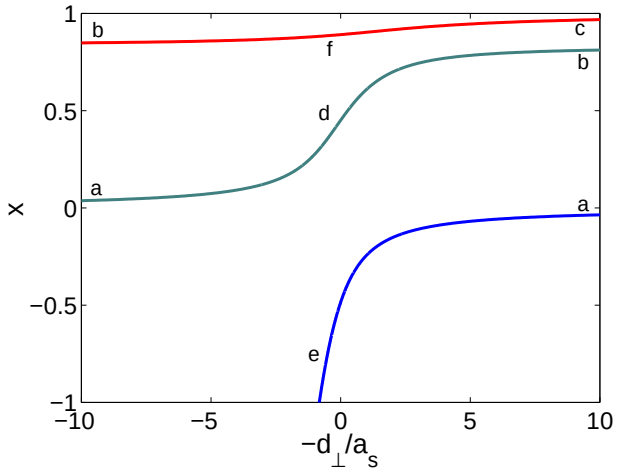


FIG. 1: (Color online) Energy spectrum of two fermions in a cylindrical harmonic trap versus inverse scattering length in the broad resonance regime. Here we choose $\lambda = 5/6$ and $|r_0|/d_\perp = 0.04$.

The energy spectrum versus inverse scattering length $-d_\perp/a_s$ for the current model is shown in Fig. 1. Across a Feshbach resonance, the scattering length can be tuned according to $a_s = a_{\rm bg}(1 - \Delta/(B - B_0))$ [24], where $a_{bg}$ is the background scattering length. $B_0$ and $\Delta$ are the resonant field and width, respectively. The effective range $r_0$ is found to satisfy $r_0 = -2\hbar^2/(m\mu a_{bg}\Delta)$ [25]. $\mu$ is the magnetic moment difference in the open and closed channel.

In this work when dealing with a broad Feshbach resonance, the validity of our model calculation requires that $|r_0| \ll d_\perp, |a_s|$. As in previous studies [22, 23], the eigenenergy remains an increasing function of the inverse scattering length $-d_\perp/a_s$. In a more complete treatment, the closed molecular channel is observed to differ from the lowest two atom (bound) state $|$e-a$\rangle$ as shown in this figure in the internal spin state [24].

## III. RESULTS ON PAIR ENTANGLEMENT

In this study, we will limit our discussion to the pair entanglement for a broad Feshbach resonance, corresponding to the regime of $|r_0| \ll d_\perp$. The nonclassical correlations (squeezing and entanglement) were previously considered for non-condensate atoms across a Feshbach resonance in free space [26]. In the following we shall

therefore focus on the two adiabatic eigenstates labelled as |a-d-b⟩ and |b-f-c⟩ in Fig. 1.

First, we briefly review the result on the molecular component according to Ref. [5]. Starting from a small positive scattering length, when adiabatically following the state |a-d-b⟩, the molecular component $P_{\rm mol} \equiv \beta^2 \ll 1$ remains small in the broad resonance regime [5, 27]. More precisely,

$$\beta^2 = \frac{|r_0|}{d_\perp} \frac{\partial x}{\partial\left(-\frac{d_\perp}{a_s}\right)}, \tag{9}$$

i.e., the molecular component is always small because of the small pre-factor $|r_0|/d_\perp$. Even smaller $P_{\rm mol}$ is expected along the state |b-f-c⟩ because it has a weaker dependence on the x-axis as shown in Fig. 1. Numerically we find that the molecular population remains less than 1% for $|r_0|/d_\perp = 0.04$.

In a spherical harmonic trap, the entanglement properties for $r_0 = 0$ have already been studied before [15]. Making use of our model as outlined above based on Ref. [5], we now extend the earlier result [15] to a cylindrical harmonic trap. To begin with, we first approximate the two fermion wave function (2) by neglecting the small molecular component, thus we obtain

$$|\Psi\rangle = \sum_{\mathbf{m},\mathbf{n}} \eta_{\mathbf{m},\mathbf{n}} a^\dagger_{\mathbf{m}\uparrow} a^\dagger_{\mathbf{n}\downarrow} |\text{vac}\rangle, \tag{10}$$

with the normalization constraint $\sum_{\mathbf{m},\mathbf{n}} |\eta_{\mathbf{m},\mathbf{n}}|^2 = 1$. $\eta_{\mathbf{m},\mathbf{n}}$ are assumed real and symmetric for two identical atoms with $\eta_{\mathbf{m},\mathbf{n}} = \eta_{\mathbf{n},\mathbf{m}}$. In the single atom basis state, the above wave function becomes

$$|\Psi\rangle = \sum_{\mathbf{m},\mathbf{n}} \eta_{\mathbf{m},\mathbf{n}} |\mathbf{m}_1 \mathbf{n}_2\rangle \frac{|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle}{\sqrt{2}}. \tag{11}$$

Such a state has both spatial and spin degrees of freedom, but the two degrees of freedom remain factorized. We therefore adopt the von Neumann entropy as our entanglement measure for a pure state. The factorized spin degree part simply contributes a ln(2), and the total entropy becomes $\mathbf{E} = \mathbf{E}_{\rm spatial} + \ln(2)$ [28]. While nontrivial, the spatial part of entanglement $\mathbf{E}_{\rm spatial}$ (abbreviated as pair entanglement) can be computed from the Schmidt decomposition [29] of the spatial wave function, i.e., we need to find

$$\sum_{\mathbf{m},\mathbf{n}} \eta_{\mathbf{m},\mathbf{n}} |\mathbf{m}\rangle_1 |\mathbf{n}\rangle_2 = \sum_{\mathbf{q}} \kappa_{\mathbf{q}} |\phi_{\mathbf{q}}\rangle_1 |\psi_{\mathbf{q}}\rangle_2, \tag{12}$$

with the Schmidt mode functions $|\phi_{\mathbf{q}}\rangle = |\psi_{\mathbf{q}}\rangle$, because $\eta_{\mathbf{m},\mathbf{n}}$ is symmetric. From this, the von Neumann entropy is found to be $\mathbf{E}_{\rm spatial} = -\sum_{\mathbf{q}} \kappa_{\mathbf{q}}^2 \ln(\kappa_{\mathbf{q}}^2)$. Computing the direct Schmidt decomposition for the three dimensional wave function turns out to be a quite demanding numerical task. Fortunately we can simplify this problem effectively to several one dimensional Schmidt decompositions, which will be discussed elsewhere [30].

For the two adiabatic states |a-d-b⟩ and |b-f-c⟩, we have numerically evaluated their spatial pair entanglement. The results are shown in Figs. 2 and 3. For both states, we find that pair entanglement is a smooth function of $-d_\perp/a_s$. The pair entanglement first increases to some maximal value, then decreases and saturates to certain finite value. The overall dependence on the atom interaction strength remains essentially the same as before [15].

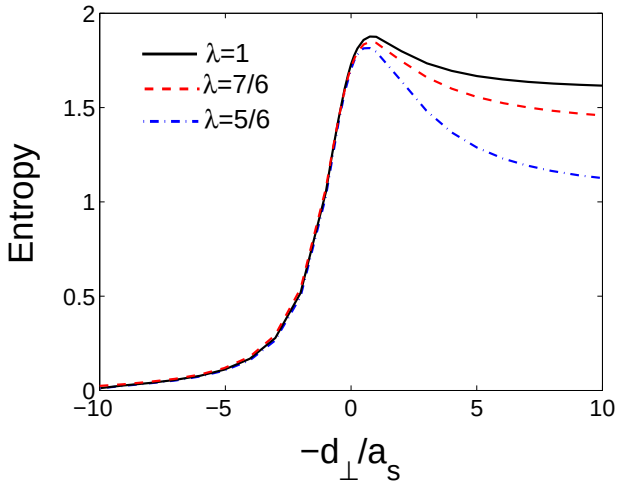


FIG. 2: (Color online) Pair entanglement versus the atomic interaction strength at different trap aspect ratio $\lambda$ for the state |a-d-b⟩ at $|r_0|/d_\perp = 0.04$. The dependence on $r_0$ is very small within the broad resonance regime.

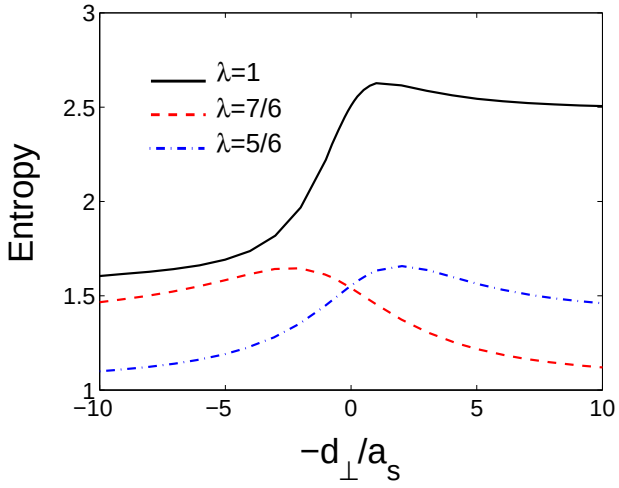


FIG. 3: (Color online) The same as in Fig. 2 except for state |b-f-c⟩.

We now discuss several interesting limits. First, for an approximately spherical trap with $\lambda \sim 1$, the adiabatic state |a-d-b⟩ corresponds to $|a\rangle$ or $|b\rangle$ at $-d_\perp/a_s \to -\infty$ or $+\infty$, respectively. For $\lambda = 5/6$, we find $|b\rangle \propto \left[\sum_{n=1,2} (c^\dagger_{nz})^2 - 2c^\dagger_{1z} c^\dagger_{2z}\right] |000\rangle_1 |000\rangle_2$,

whose pair entanglement is $\ln(2\sqrt{2}) \approx 1.04$. Here we again follow the notation of Ref. [5] with $c^\dagger_{nj}$ the creation operator for a fermionic atom indexed by $n$ in the $j$-th trap direction. State $|m_1 m_2 m_3\rangle_n$ therefore refers to atom $n$ in the motional state $m_j$ along the $j$-th direction. For $\lambda = 7/6$, we find $|b\rangle \propto \left[\sum_{n=1,2;j=x,y}(c^\dagger_{nj})^2 - 2\sum_{j=x,y} c^\dagger_{1j}c^\dagger_{2j}\right]|000\rangle_1|000\rangle_2$ with a pair entanglement $\ln(4) \approx 1.39$. For $\lambda = 1$, we find $|b\rangle \propto \left[\sum_{n=1,2;j=x,y,z}(c^\dagger_{nj})^2 - 2\sum_{j=x,y,z} c^\dagger_{1j}c^\dagger_{2j}\right]|000\rangle_1|000\rangle_2$ with a pair entanglement $\ln(2\sqrt{6}) \approx 1.59$. We find that the pair entanglement is always larger at the limit of a spherical trap with $\lambda = 1$. For the adiabatic state $|$b-f-c$\rangle$, we find generally that the pair entanglement at $\lambda = 1$ is well separated from $\lambda \neq 1$ because of the increased motional state degeneracy. State $|c\rangle$ corresponds to the limit of $-d_\perp/a_s \to +\infty$, which for $\lambda = 7/6$ becomes $|c\rangle \propto \left[\sum_{n=1,2}(c^\dagger_{nz})^2 - 2c^\dagger_{1z}c^\dagger_{2z}\right]|000\rangle_1|000\rangle_2$, which is precisely the state $|b\rangle$ for $\lambda = 5/6$ in the adiabatic state $|$a-d-b$\rangle$, whose pair entanglement therefore remains the same $\ln(2\sqrt{2}) \approx 1.04$. This correspondence persists also for $\lambda = 5/6$, where the state $|c\rangle$ is the same as state $|b\rangle$ for $\lambda = 7/6$ in the adiabatic state $|$a-d-b$\rangle$. The state $|c\rangle$ at $\lambda = 1$ is more complicatedly expressed as a linear combination of different single particle states as $|c\rangle \propto \left[ -\sum_{n=1,2;j=x,y,z}(c^\dagger_{nj})^4 - \sum_{n,m;j\neq k}(c^\dagger_{mj})^2(c^\dagger_{nk})^2 - 6\sum_j (c^\dagger_{1j})^2(c^\dagger_{2j})^2 + 4\sum_{n\neq m;j} c^\dagger_{mj}(c^\dagger_{nj})^3 + 4\sum_{n;j\neq k} c^\dagger_{1j}c^\dagger_{2j}(c^\dagger_{nk})^2 - 8\sum_{j\neq k} c^\dagger_{1j}c^\dagger_{1k}c^\dagger_{2j}c^\dagger_{2k}\right]|000\rangle_1|000\rangle_2$, whose pair entanglement is $55\ln(2)/24 + 7\ln(3)/8 - \ln(5)/24 \approx 2.48$.

We next consider two extreme cases of $\lambda \ll 1$ or $\lambda \gg 1$ corresponding to the quasi-one- and quasi-two-dimensional limits, respectively [22]. The pair entanglement results are shown in Fig. 4 for both $\lambda = 1/20$ and $\lambda = 20$. We find that the pair entanglement saturates to a lower value in the quasi-one-dimensional limit at $\lambda = 1/20$, again because of the reduced motional state degeneracy. Our results here are of course limited to the validity regime of the model we adopt in the Hamiltonian (1). For a more rigorous treatment, please refer to the methods developed in Ref. [31] for harmonic traps or atomic waveguides.

## IV. A TOY MODEL

Much of our results above can in fact easily be appreciated from a toy model for two distinguishable atoms, as described by the Hamiltonian $H = H_0 + V$, with $H_0$ and $V$ given by

$$\begin{aligned} H_0 &= \hbar\omega(|10\rangle_{12}\langle 10| + |01\rangle_{12}\langle 01|), \\ V &= \hbar\delta|00\rangle_{12}\langle 00| \\ &\quad +\hbar\eta(|10\rangle_{12}\langle 00| + |01\rangle_{12}\langle 00| + \text{h.c.}). \end{aligned} \quad (13)$$

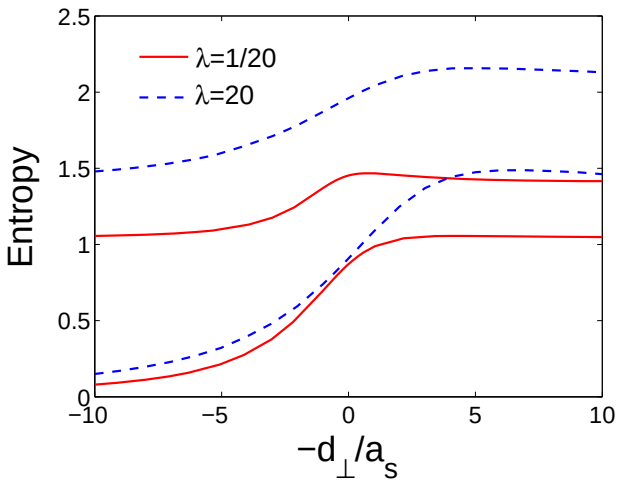


FIG. 4: (Color online) Entropy as function of inverse scattering length for processes $|$a-d-b$\rangle$ and $|$b-f-c$\rangle$. Red solid lines are for $\lambda = 1/20$, and blue dashed lines are for $\lambda = 20$. The corresponding lower one is for process $|$a-d-b$\rangle$, while the upper one is for $|$b-f-c$\rangle$.

For simplicity, we have truncated the motional states to only include the ground and the first excited state, denoted respectively by $|0\rangle$ and $|1\rangle$ and separated by the trap frequency $\omega$. The collisional interaction is mainly limited to the ground state manifold, giving rise to a level shift $\delta$ when both atoms are in the ground state ($|00\rangle$) and a simple atom excitation with strength $\eta$. Double excitation is assumed small and neglected.

This toy model can be easily solved, and the pair entanglement as function of interaction parameter $\eta/(\omega-\delta)$ is shown in Fig. 5. We see that the ground state is a simple product state of each atom in the motional state $|0\rangle$ for $\eta = 0$, i.e., displaying no entanglement. With the increase of atom-atom interaction, we find that the entanglement increases and saturates to $2\ln(2) - \frac{\sqrt{3}}{2}\ln(2+\sqrt{3}) \simeq 0.2458$, where the approximations for the toy become questionable.

It is important to note that this toy model reproduces the same dependence of pair entanglement on the interaction strength as for the system of two fermionic atoms during the BCS to BEC crossover. We thus feel it is important to point out that from the point of view of two atom motional state entanglement, nothing particularly significant occurs during the BCS to BEC crossover.

## V. CONCLUSION

Before concluding, let us briefly summarize the generalization of our current study to a narrow Feshbach resonance, where the bound state molecular component in Eq. (2) cannot be neglected anymore. The pair entanglement inside the molecular component can be included by performing an analogous symmetric Schmidt decom-

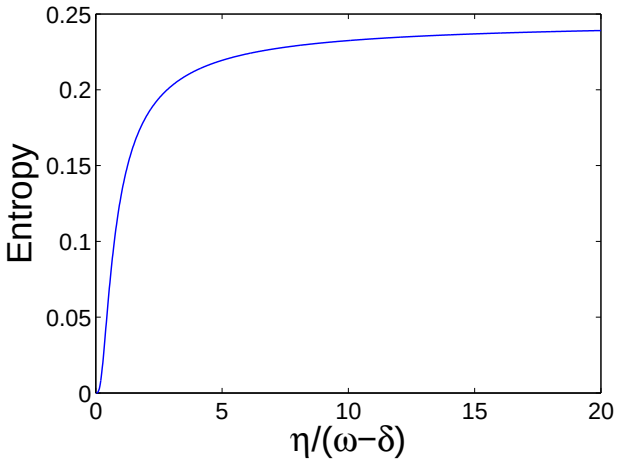


FIG. 5: (Color online) The dependence of pair entanglement as a function of interaction parameter $\eta/(\omega - \delta)$.

position on Eq. (2). The total pair correlation can then be computed analogously in terms of the entropy of the independent Schmidt orbital expansion. Of course, such an approach would require more details about the model formulation and the exact determination of the molecular bound state wave function.

In summary, we have studied pair entanglement between two spin-1/2 fermionic atoms inside a single optical lattice site approximated by a cylindrical harmonic trap. We investigated thoroughly the dependence of pair entanglement on the trap strength and geometry and on atom-atom interaction strength along the complete BCS to BEC crossover and focused on the broad resonance regime. We developed a formalism for studying pair entanglement including the effect of an effective range $r_0$ for two interacting atoms at low energy. In the limit of a broad Feshbach resonance, where the effect of $r_0$ becomes negligibly small, our result reduces to the theory developed before for evaluating pair entanglement in a single open channel of two atoms without the presence of a bound molecule state. We find that pair entanglement changes significantly against atomic pair interaction because of the induced motional orbital deformations. In general, however, the exact value of the spatial pair entanglement is also governed by the motional state degeneracies. As a rule of thumb, we find that spherical harmonic traps generally give rise to larger pair entanglement. We hope our study will provide new insights into the applications of quantum degenerate lattice systems to quantum information science.

## VI. ACKNOWLEDGEMENT

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